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1.INTRODUCTION

Several studies have been communicated in recent years considering nano-coating protective layers for gas turbine environments. They have generally shown that improved protection is achieved compared with conventional thermal barrier coatings (TBCs) which are susceptible to various life limiting issues associated with their operating environment including erosion, corrosion, oxidation, sintering and foreign object damage (FOD) [1,2]. Nano-coatings engineered for high temperature applications have been investigated for surface roughness and topography, residual stress, adherence, damage tolerance and resistance, tribological properties, lubrication, coefficient of friction and hot hardness. Motivated by these developments, in this presentation we describe recent finite element thermal stress simulations of nano-coated (Aluminium Oxide/Titanium Oxide metallic nano-particle mix). The simulations demonstrate that largely due to the higher thermal conductivity and smaller size of nano-particles, they achieve improved bonding in coatings and dissipate heat better than conventional micro-coatings. Greater integrity of the coating is achieved and lower susceptibility to corrosion gas penetration is obtained with nano-coatings compared with micro-coatings. ANSYS Workbench version 19.1 [3] has been employed to simulate the thermal stress response of nano-coatings. Extensive visualization of results is included. Important deductions on nano-coating performance are made. The study provides a useful compliment to experimental tests which are also being conducted.

2. NANO-COATING PROPERTIES

Since a continuum-based finite element approach is adopted, molecular variations in nano-particle dynamics in the coating cannot be simulated. Instead an *average value of materials properties* is adopted for a 60:40 % titanium oxide (TiO_2) : aluminium oxide (Al_2O_3) mix nano-coating (powder). The table below summarizes the key material properties (Young modulus, Poisson ratio, density and thermal conductivity) for the original nano—powders and the composite nano-coating:

Property	Steel (AISI 304 Superalloy)	Titanium oxide (nano-powder)	Alumina (Aluminium oxide nano-powder)	Nano-coating Alumina-Titanium Oxide 60:40 mix
Young Modulus	200GPa	288 GPa	413GPa	363 GPa
Poisson Ratio	0.28	0.29	0.33	0.314
Density	7850kg/m ³	4050kg/m ³	3980 kg/m ³	4008 kg/m ³
Thermal conductivity	50W/mK	20W/mK	24W/mK	9.6W/mK

3. ANSYS THERMAL STRESS FORMULATION

In ANSYS to simulate coupled thermal stress analysis, the stresses are related to the strains as follows [3]:

$$\{\sigma\} = [D] \{\epsilon^{el}\}$$

$\{\sigma\}$ = Stress Vector
 $[D]$ = Elastic or elastic stiffness matrix
 $\{\epsilon^{el}\}$ = Elastic strain vector
 $\{\epsilon\}$ = Total strain vector
 $\{\epsilon^{th}\}$ = Thermal strain vector

For the 3-dimensional analysis, thermal strain vector takes the form:

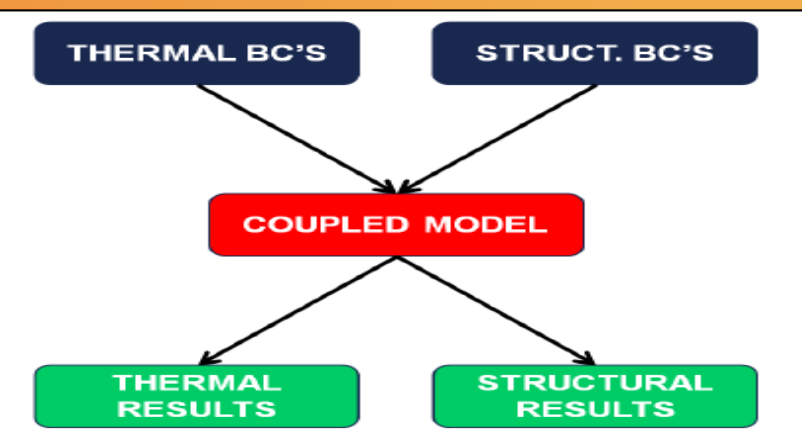
$$\{\epsilon^{th}\} = \Delta T \begin{bmatrix} \alpha_x & \alpha_y & \alpha_z & 0 & 0 & 0 \end{bmatrix}^T$$

The element integration point strains and stresses are computed by combining the following two equations:

$$\{\epsilon^{el}\} = [B] \{u\} - \{\epsilon^{th}\}$$

$$\{\sigma\} = [D] \{\epsilon^{el}\}$$

$\{\epsilon^{el}\}$ = Strains
 $[B]$ = Strain – displacement matrix evaluated at integration point
 $\{u\}$ = Nodal displacement vector
 $\{\epsilon^{th}\}$ = Thermal strain vector
 $\{\sigma\}$ = stress vector
 $[D]$ = Elasticity matrix

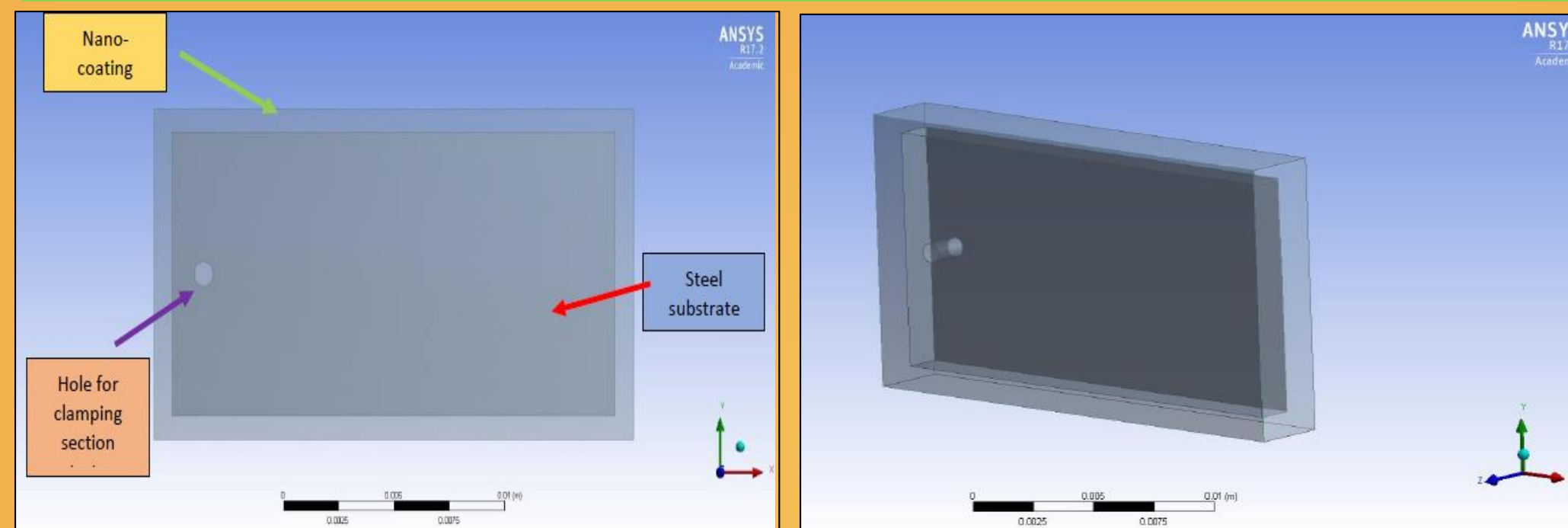


α_x = thermal coefficient of expansion in the x direction (1/K)
 ΔT = $T - T_{REF}$ (K)
 T = current temperature (K)
 T_{REF} = reference (strain – free) temperature

Fourier heat conduction assumed

4. ANSYS MESH AND THERMAL STRESS ANALYSIS

A three-dimensional model was created using the ANSYS static structural geometry modeller to represent a steel sample under high temperature corrosion. A two-layered domain in (x,y,z) space is created with the base layer representing the gas turbine blade substrate (AISI 304 super alloy) and the upper layer simulating the Alumina-Titanium oxide nano-coating, as shown below. Note the nano-coating completely engulfs the substrate specimen. The fixture (cylindrical hole) is also shown in order to compare simulations with future HVOF experiments. Below shows the front (top) and 3-D rendition of the model. The clamping is achieved via the hole which penetrates the entire substrate and is filled with nano-material during the coating process. The nano coating thickness is 0.816 mm. The substrate sample dimensions are 10.98mm (depth), 20.76mm (length) and width (186mm). The boundary conditions imposed on all six faces of the coated model is a thermal one due to the hot gas at an average temperature of 1000 °C. The structural boundary condition is the fixing hole where the model is constrained.



The von Mises or equivalent stress σ_e (output as SEQV) is computed as:

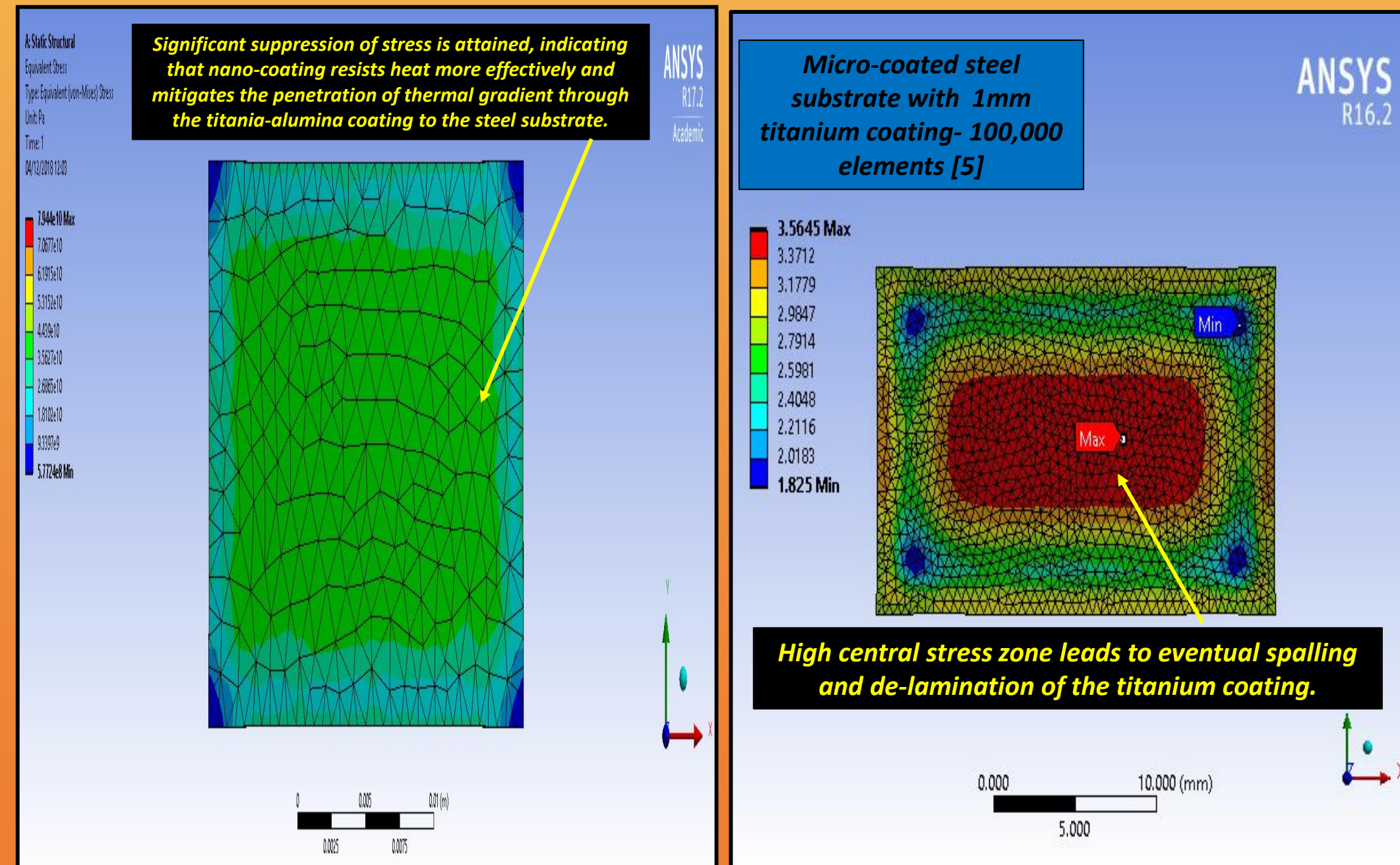
$$\sigma_e = \text{MAX}(|\sigma_1 - \sigma_2|, |\sigma_2 - \sigma_3|, |\sigma_3 - \sigma_1|)$$

The equivalent stress is related to the equivalent strain ϵ_e through:

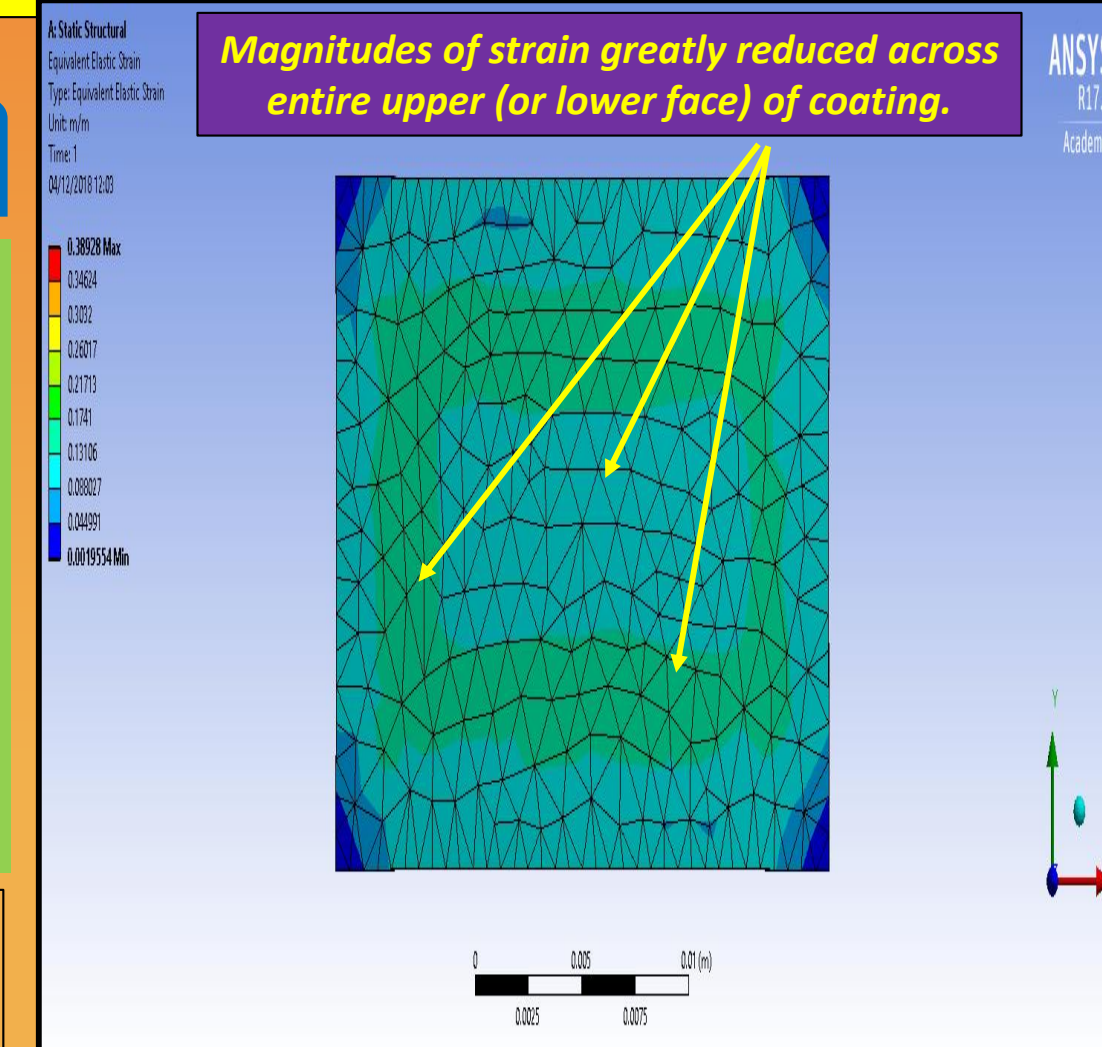
$$\sigma_e = E \epsilon_e$$

E= Young's modulus (input as EX on MP command)

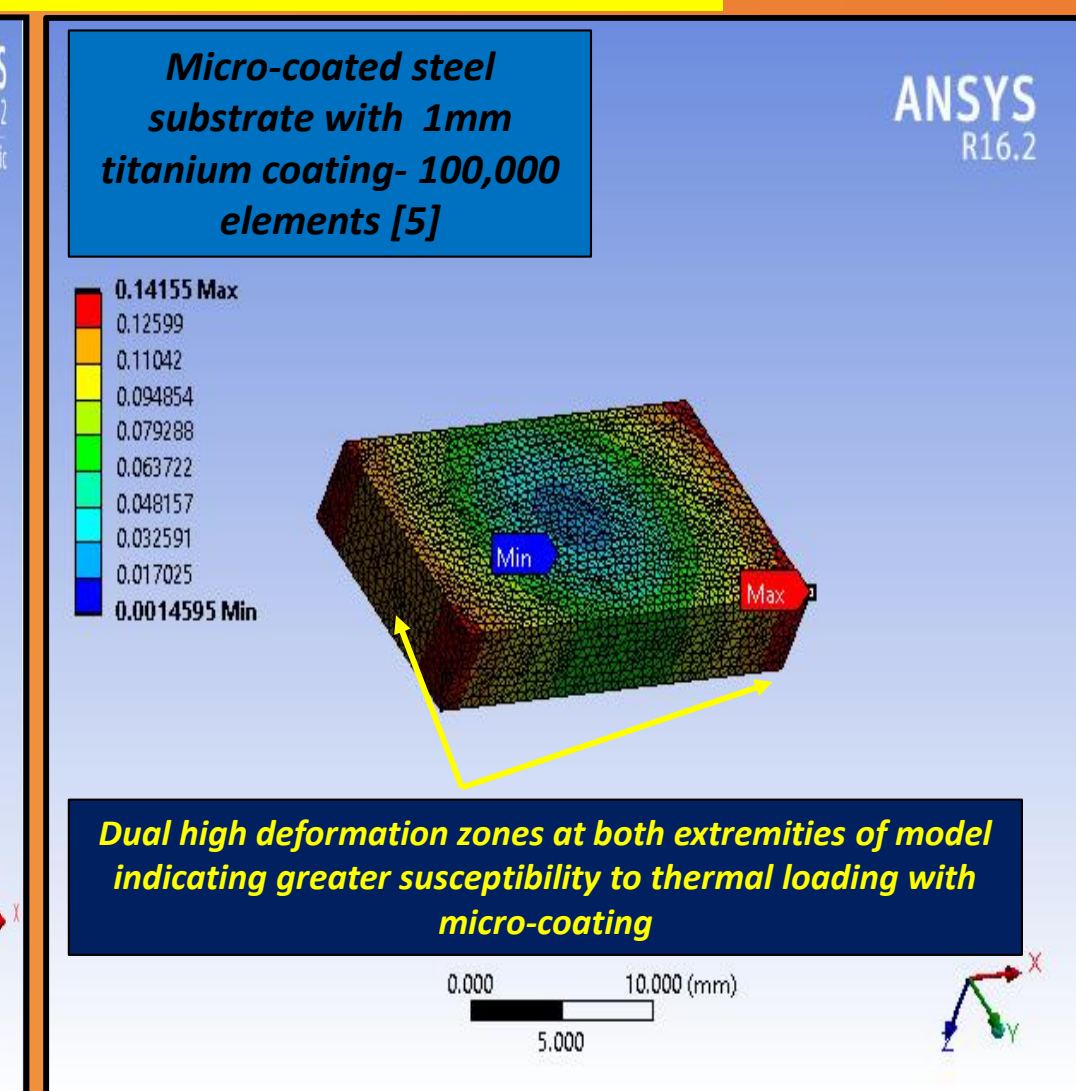
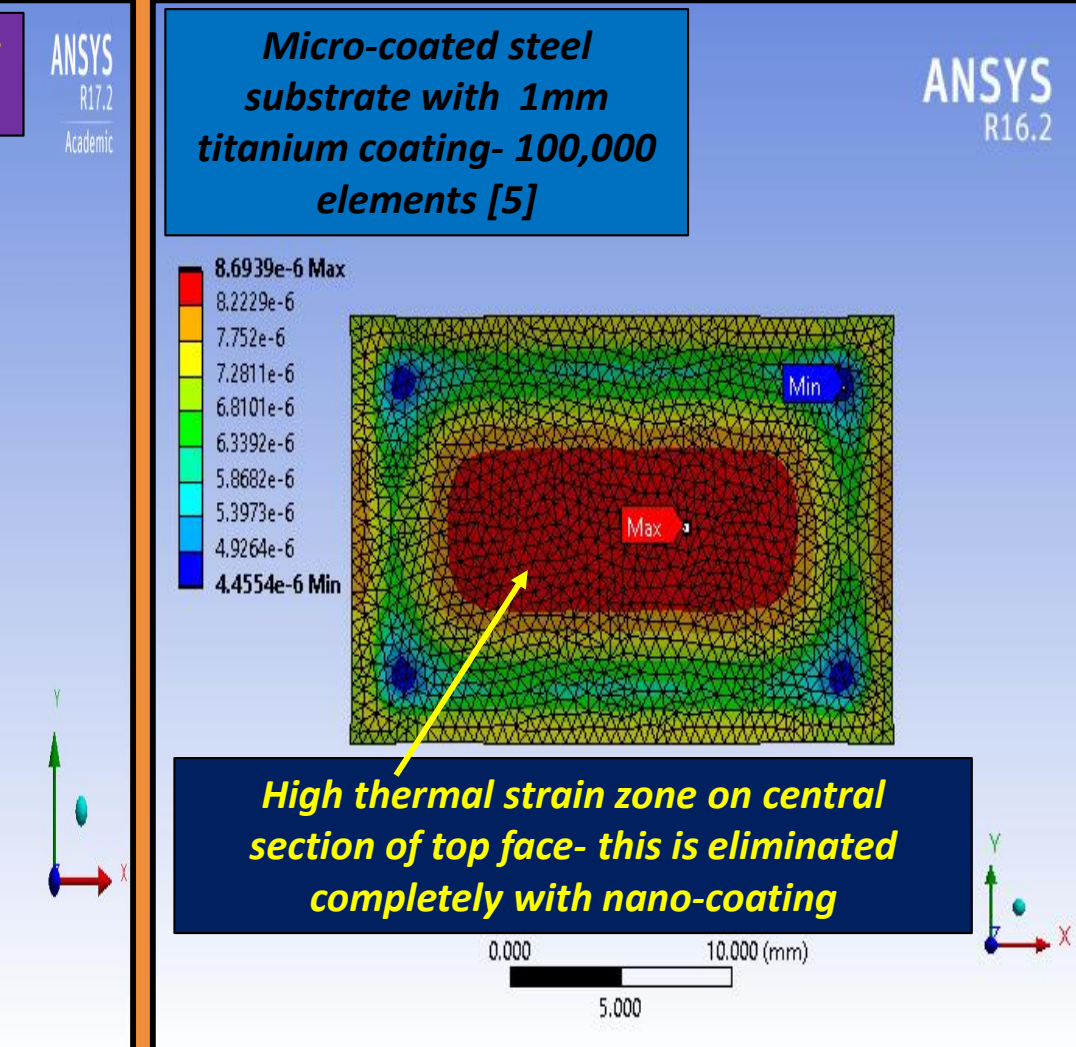
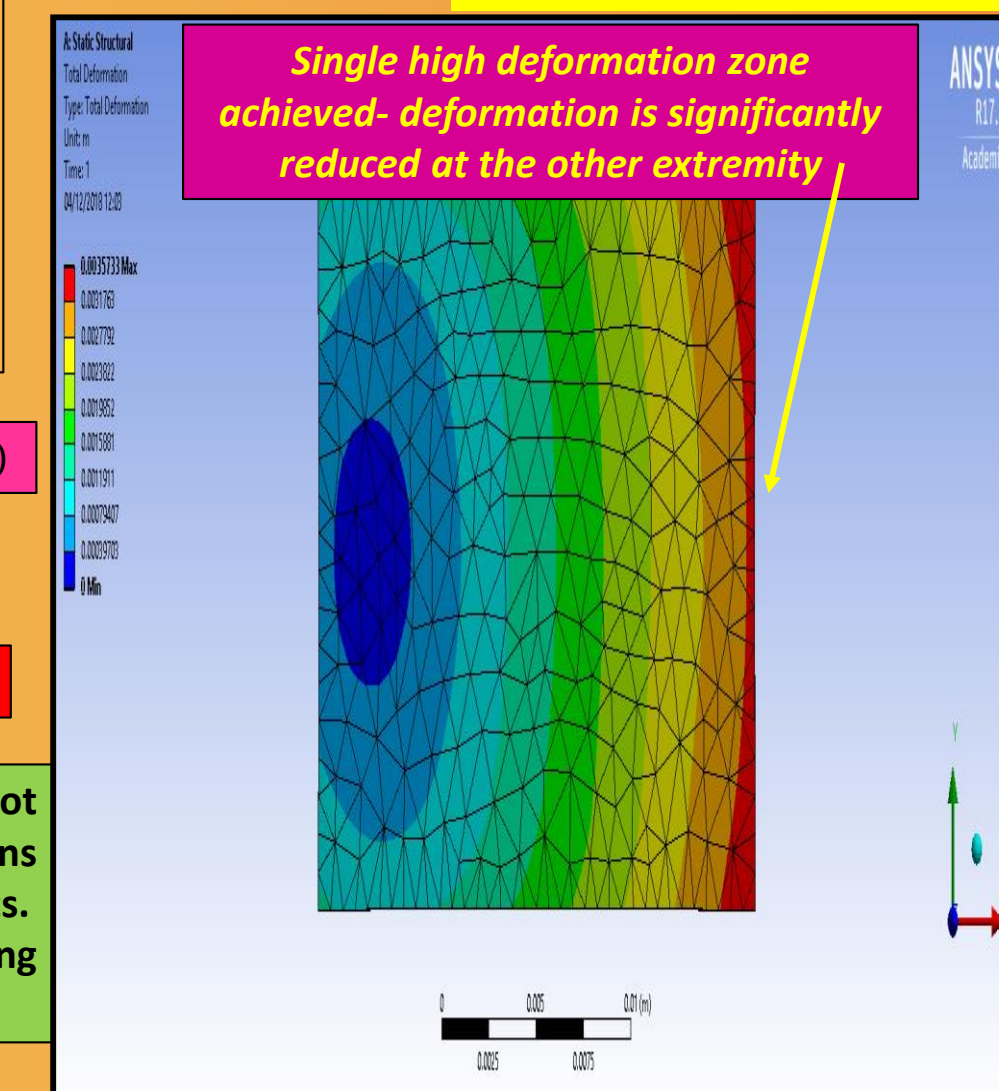
N.B. In ANSYS workbench, the data is usually supplied as a mean value and this data is correctly used by ANSYS, if T_{REF} is not only the definition temperature about which the data is supplied but also the reference temperature at which zero strains exist. Mesh independence was tested for. A default mesh of 140,000 elements was found to achieve grid independent results. The nano-coating simulations are compared with micro-coated steel samples using a single Titanium thermal barrier coating layer also engulfing the sample with 1mm depth, performed in an earlier study [4].



Equivalent stress - 60:40 Alumina-Titanium oxide nano-coating versus micro-coated titanium case



Equivalent strain -60:40 Alumina-Titanium oxide nano-coating versus micro-coated titanium case



Total deformation plot for 60:40 Alumina-Titanium oxide nano-coating versus micro-coated titanium case

5. CONCLUSIONS

In all cases the nano-coating is found to provide superior thermal protection to the steel substrate (AISI 304 super alloy). High stress zones are completely eliminated with nano-coating whereas they are prevalent with titanium micro-coating. Although titanium oxide has excellent thermal resistance properties, the alumina nano-powder when mixed with titania, produces an inert performance which is and resistant to inter-diffusion and this leads to stability during exposure to elevated temperatures for long periods of time, thus preserving the sharp interface and minimizing thermal stresses which are necessary for good thermal barrier performance. The alumina material tends to form an amorphous structure when it is deposited onto a substrate which is held at a relatively low temperature and in the alternative it tends to form a crystalline structure when applied by a vapor deposition to a substrate held at a relatively high temperature. Either case will result in a very resilient nano-coating which achieves excellent bonding to the super alloy substrate and prevents the penetration of hot gas since at the nanoscale cracks of micro-scale magnitude are mitigated. This is not possible in the micro-coating which flakes, permits heat penetration, has reduced integrity and eventually cracks. Alumina being integral to the coating layer and in contact with the substrate has the desirable characteristic that since the native oxide which forms on the substrate due to oxidation of the substrate will be alumina, therefore having a nano-structured alumina layer in the coating adjacent to a naturally occurring alumina layer will probably provide the best coating adherence as noted in [2]. Overall much lower stresses, strains and deformations are produced with nano-coatings compared with micro-coatings.

REFERENCES

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